ELECTRONIC SUPPLETARY INFORMATION (ESI)

Synthesis and structural characterization of homochiral 2D coordination polymers of zinc and copper with conformationally flexible ditopic imidazolium-based dicarboxylate ligands

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Table S1. Crystal data and structure refinement for compounds **2**, **4**-**6** and **8** from single-crystal X-ray crystallography.

	2	**4**	**5**	**6**	**8**
Formula	$C_{52}H_{76}N_8O_{16}Zn_2$	$C_{48}H_{54}N_6O_{11}Zn$	$C_{18}H_{22}CuN_4O_8$	$C_{26}H_{38}CuN_4O_8$	$C_{126}H_{114}Cu_3N_{12}O_{24}$
M	1199.99	956.34	485.93	598.14	2370.91
T [K]	193(2)	193(2)	193(2)	193(2)	193(2)
Wavelength [Å]	0.71073	0.71073	0.71073	0.71073	0.71073
Crystal system	Orthorhombic	Trigonal	Orthorhombic	Triclinic	Orthorhombic
Space group	P 2_1 2_1 2_1	P 3_2	P 2_1 2_1 2	P 1	C 2 2 2_1
a [Å]	13.1331(16)	10.5395(2)	13.7058(10)	6.7462(8)	14.8008(3)
b [Å]	19.104(2)	10.5395(2)	14.2753(10)	10.0831(11)	26.4440(5)
c [Å]	24.643(2)	36.9255(11)	10.3260(7)	10.6524(12)	33.4891(6)
α [°]	90	90	90	87.226(4)	90
β [°]	90	90	90	83.190(4)	90
γ [°]	90	120	90	86.503(4)	90
V [Å^3]	6182.9(11)	3552.20(14)	2020.3(2)	717.53(14)	13107.4(4)
Z	4	3	4	1	4
$D_{calcd.}$ [Mg·m^{-3}]	1.289	1.341	1.598	1.384	1.201
μ [mm^{-1}]	0.844	0.584	1.136	0.814	0.552
F(000)	2528	1506	1004	315	4932
Crystal size [mm^3]	0.50 x 0.40 x 0.40	0.50 x 0.50 x 0.40	0.50 x 0.50 x 0.40	0.40 x 0.40 x 0.20	0.50 x 0.40 x 0.30
Theta range for data collection [°]	1.65 to 25.25	1.10 to 25.24	1.97 to 30.52	1.93 to 25.25	1.66 to 25.25

Index ranges	$-11 \le h \le 15$, $-22 \le k \le 17$, $-29 \le l \le 29$	$-11 \le h \le 12$, $-12 \le k \le 12$, $-44 \le l \le 44$	$-19 \le h \le 19$, $-13 \le k \le 20$, $-13 \le l \le 9$	$-8 \le h \le 8$, $-12 \le k \le 11$, $-10 \le l \le 12$	$-17 \le h \le 17$, $-23 \le k \le 31$, $-40 \le l \le 23$
Reflections collected	56025	39974	23225	11676	58137
Independent reflections	11097 [R(int) = 0.0926]	8447 [R(int) = 0.0253]	5249 [R(int) = 0.0202]	3678 [R(int) = 0.0344]	11758 [R(int) = 0.0244]
Completeness to theta %	99.9	100.0	92.9	98.2	99.7
Absorption correction	Semi-empirical from equivalents				
Max. and min. transmission	0.7289 and 0.6777	0.7998 and 0.7587	0.6593 and 0.6004	0.8541 and 0.7366	0.8520 and 0.7700
Refinement method	Full-matrix least-squares on F^2				
Data / restraints / parameters	11097 / 36 / 703	8447 / 19 / 606	3559 / 0 / 286	3678 / 3 / 361	11758 / 543 / 764
Goodness-of-fit on F^2	1.032	1.057	0.995	1.043	0.821
Final R indices [$I>2\sigma(I)$]	R1 = 0.0919, wR2 = 0.2329	R1 = 0.0369, wR2 = 0.1054	R1 = 0.0192, wR2 = 0.0517	R1 = 0.0765, wR2 = 0.2049	R1 = 0.0475, wR2 = 0.1691
R indices (all data)	R1 = 0.1073, wR2 = 0.2496	R1 = 0.0373, wR2 = 0.1057	R1 = 0.0217, wR2 = 0.0563	R1 = 0.0774, wR2 = 0.2063	R1 = 0.0537, wR2 = 0.1800
Absolute structure parameter	-0.02(2)	0.029(4)	0.005(11)	0.10(3)	0.047(16)
Largest diff. peak and hole [$e \cdot Å^{-3}$]	1.942 and -1.431	0.450 and -0.315	0.242 and -0.376	3.461 and -1.119	0.828 and -0.529

Table S2. Crystal data and structure refinement for compounds **3** and **7** from X-ray powder diffraction.

	3	**7**
Formula	$C_{52}H_{76}N_8O_{16}Zn_2$	$C_{26}H_{38}CuN_4O_8$
M	1199.99	598.14
T [K]	293	293
Wavelength [Å]	1.5406	1.5406
Crystal system	orthorhombic	triclinic
Space group	P 2_1 2_1 2_1	P 1
a [Å]	13.2622(14)	6.8273(6)
b [Å]	19.1377(32)	10.0864(10)
c [Å]	24.7652(18)	10.6764(10)
α [°]	90.0	86.830(9)
β [°]	90.0	83.672(9)
γ [°]	90.0	86.901(7)
V	6285.6(11)	728.76(15)
Z	8	1
$V_{\text{non-H-atom}}$ [Å^3]	10.07	18.68
Independent reflections	2127	2202
Data / restraints / parameters	3905/172/268	5821/89/147
R_{WP}	0.0789	0.0494
R_P	0.0549	0.0363
R_F	0.0465	0.0410

- Fig. S1. Supramolecular 3D packing in compound $[Zn((S,S)\text{-}L^{iPr})_2 \cdot H_2O]_n$, **2**, with three 2D lamellar sheets, viewed along *b* axis.

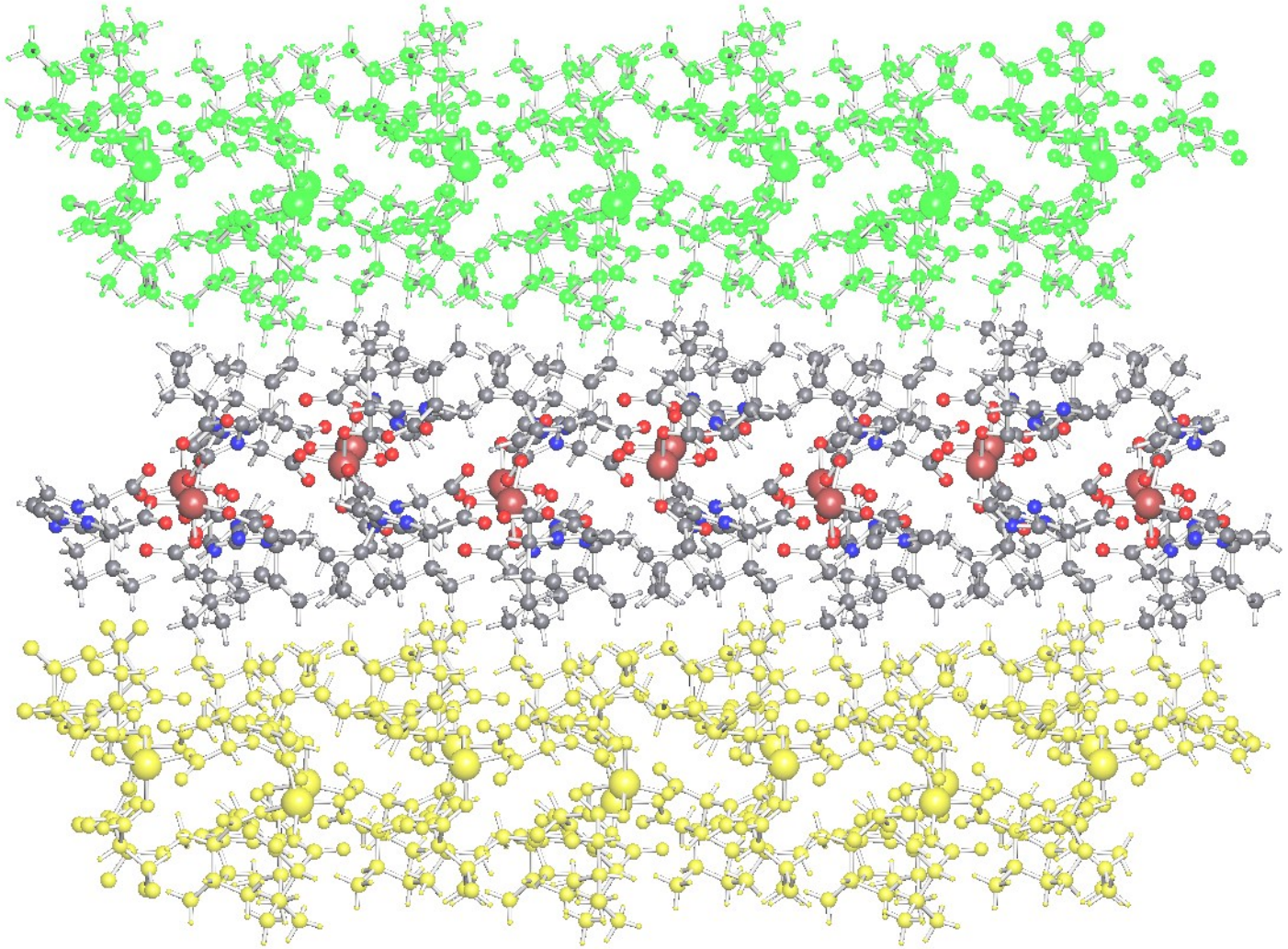


Fig. S2. Final observed (crosses), calculated (solid line) and difference plot for the Rietveld refinement of complex $[Zn((R,R)\text{-}L^{iPr})_2 \cdot H_2O]_n$ (**3**). The inset shows a zoom of the 10 - 40° 2θ region.

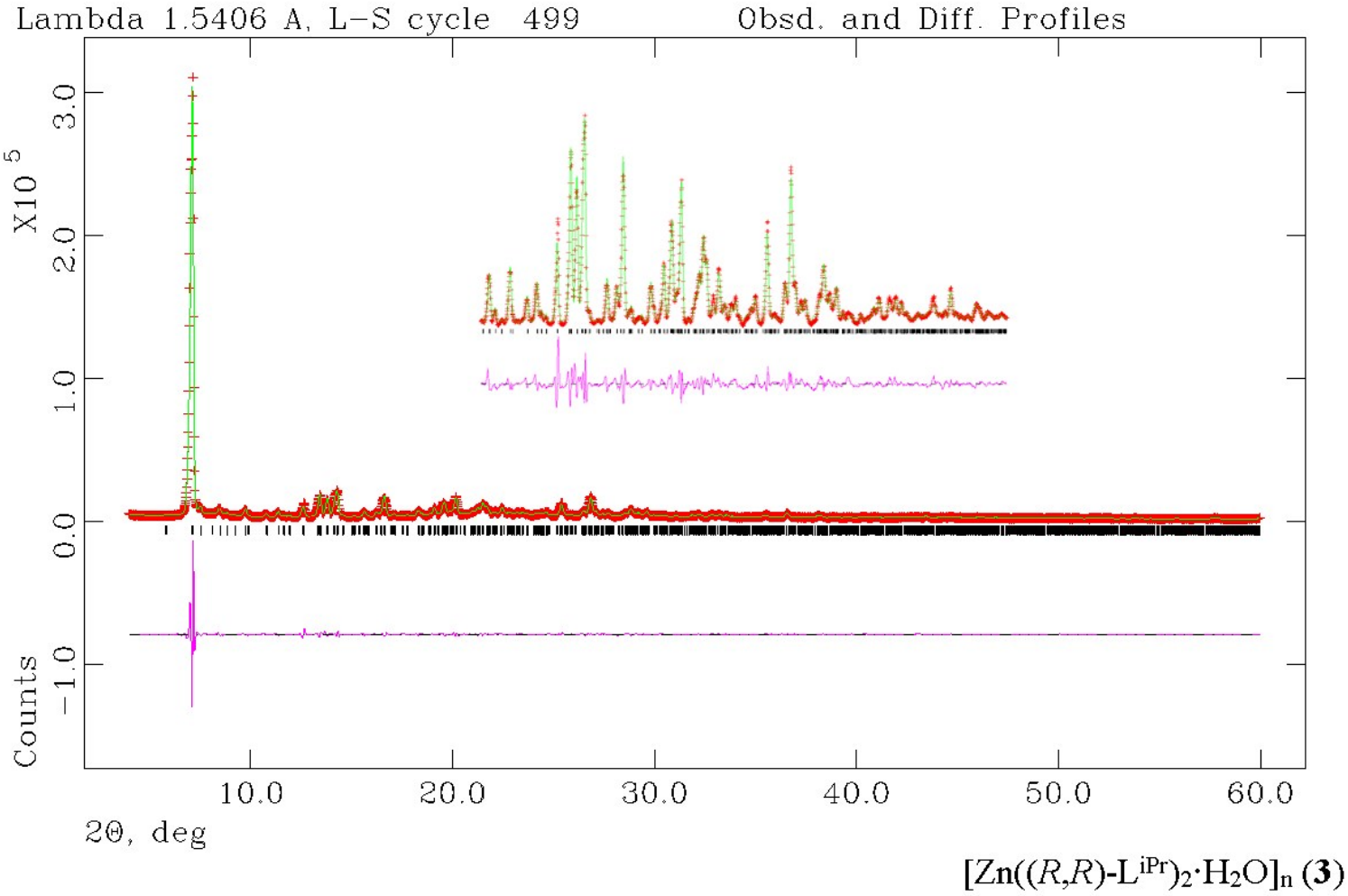
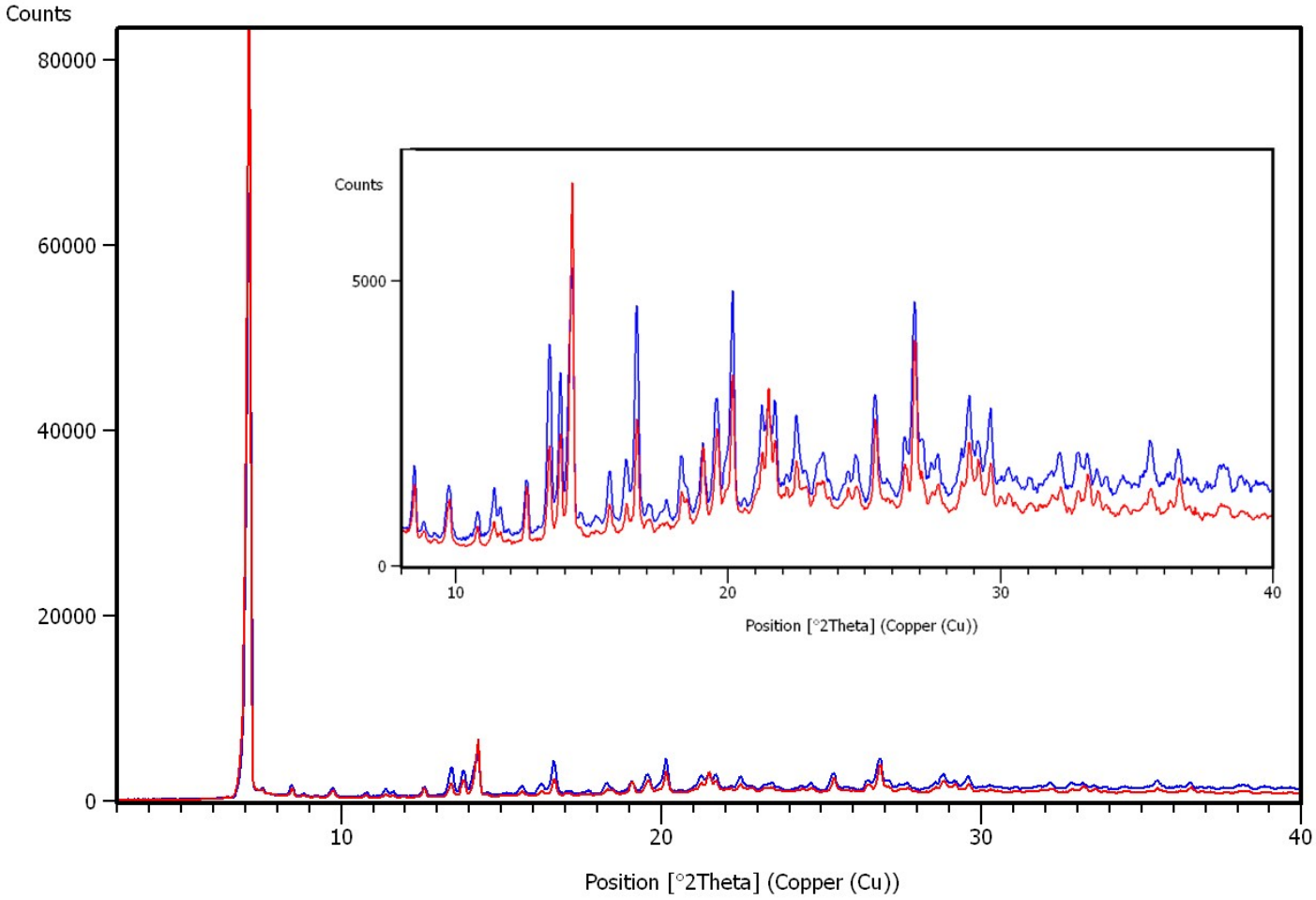


Fig. S3. Comparison of the XRPDs for complexes $[Zn((S,S)\text{-}L^{iPr})_2 \cdot H_2O]_n$ (**2**) (red) and $[Zn((R,R)\text{-}L^{iPr})_2 \cdot H_2O]_n$ (**3**) (blue). The inset shows a zoom of the 10 - 40° 2θ region.



- Fig. S4. Supramolecular arrangement of six 2D sheets of complex $[Cu((S,S)\text{-}L^{iPr})_2]_n$, **6**, viewed along *b* axis.

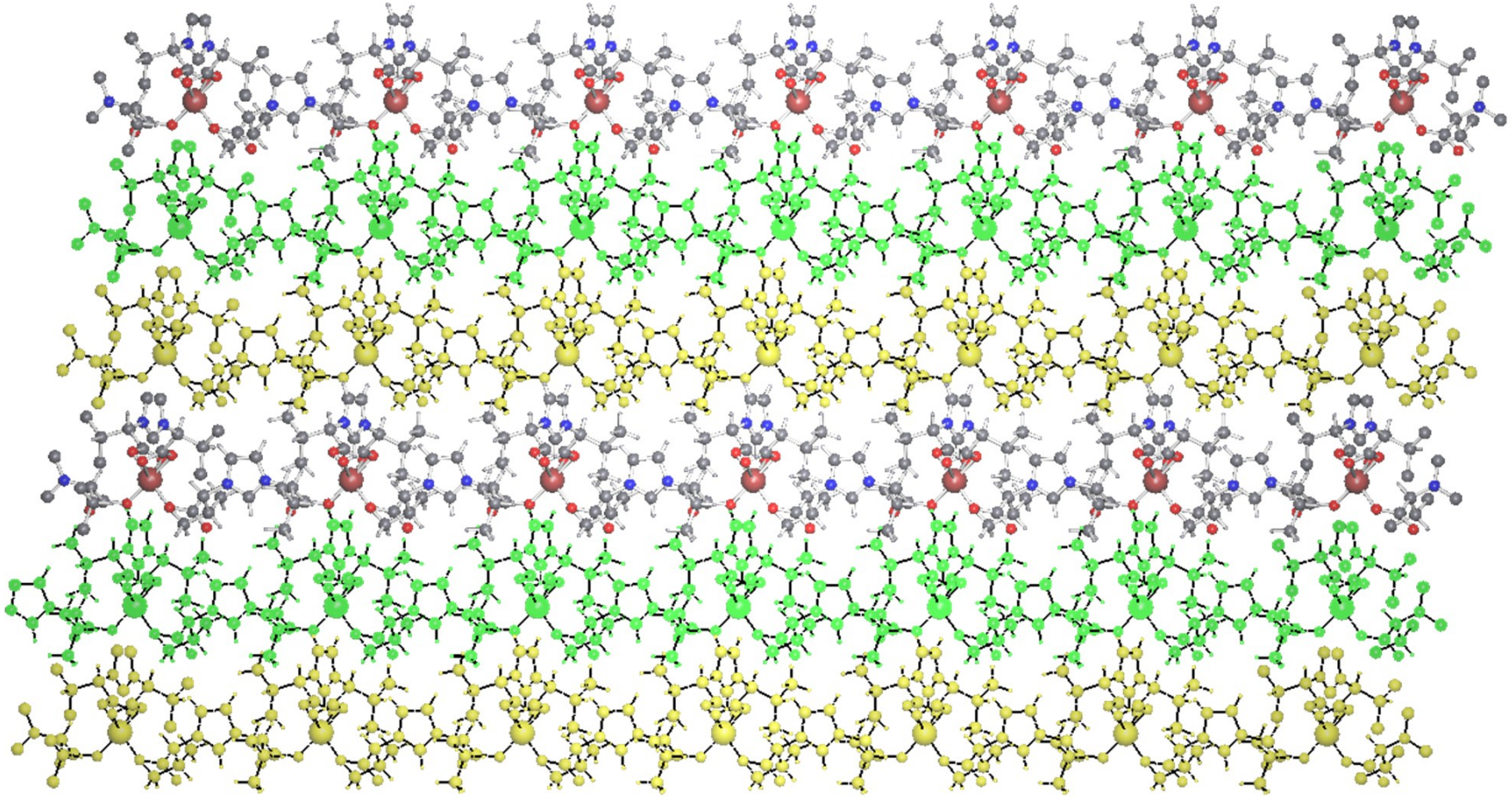


Fig. S5. Comparison of the XRPDs for complexes $[Cu((S,S)\text{-}L^{iPr})_2]_n$ (**6**) (red) and $[Cu((R,R)\text{-}L^{iPr})_2]_n$ (**7**) (blue).

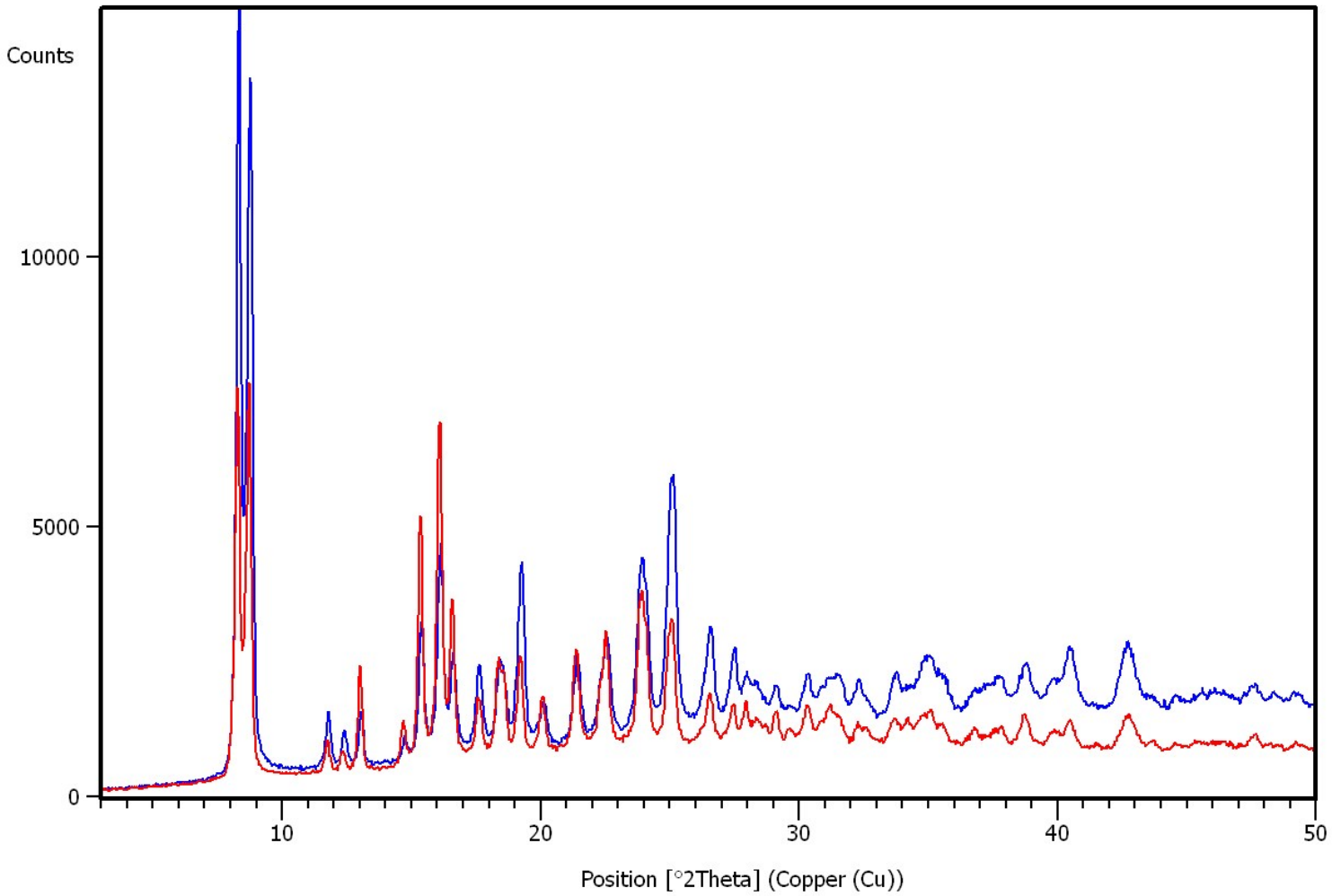
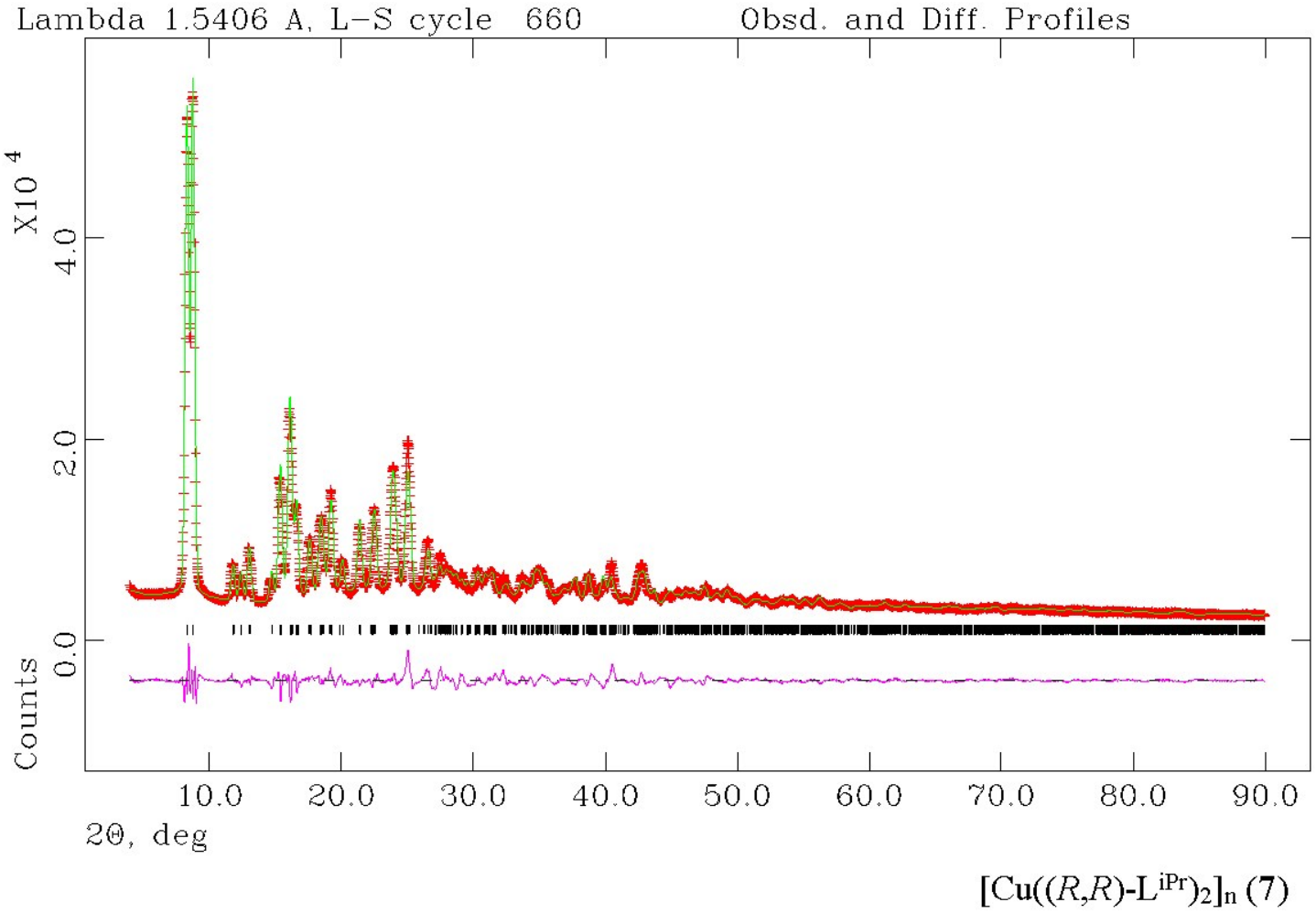
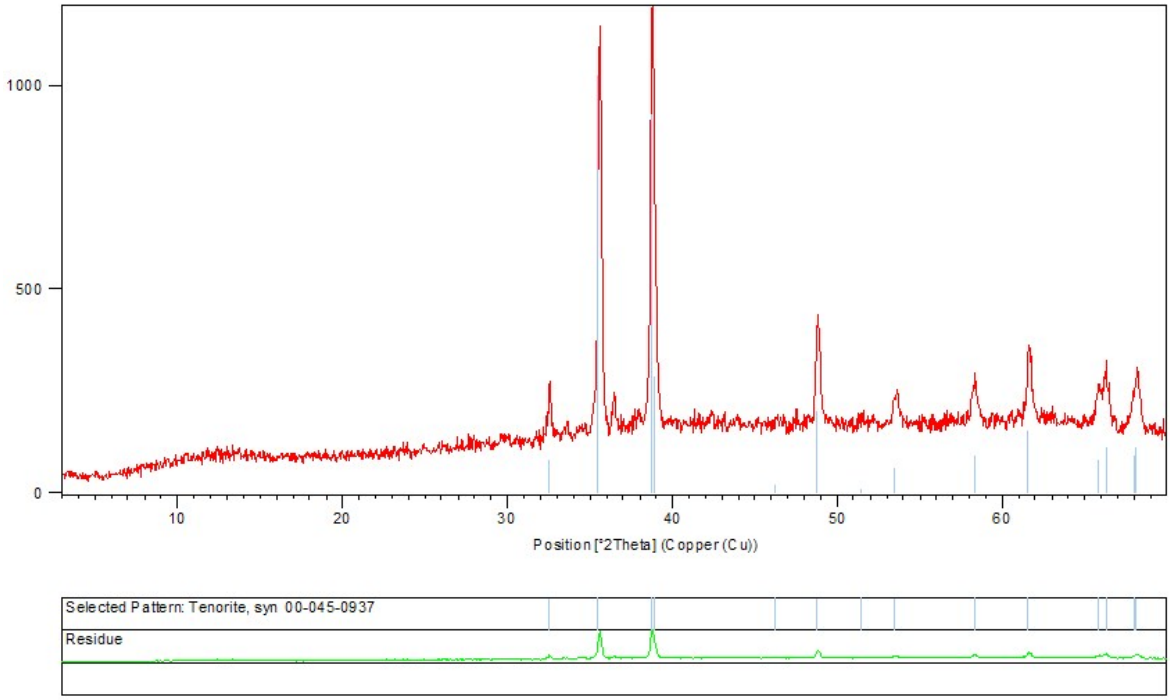


Fig. S6. Final observed (crosses), calculated (solid line) and difference plot for the Rietveld refinement of complex $[Cu((R,R)\text{-}L^{iPr})_2]_n$ (**7**).



- Fig. S7. Identification of the TGA residue as CuO by PXRD.

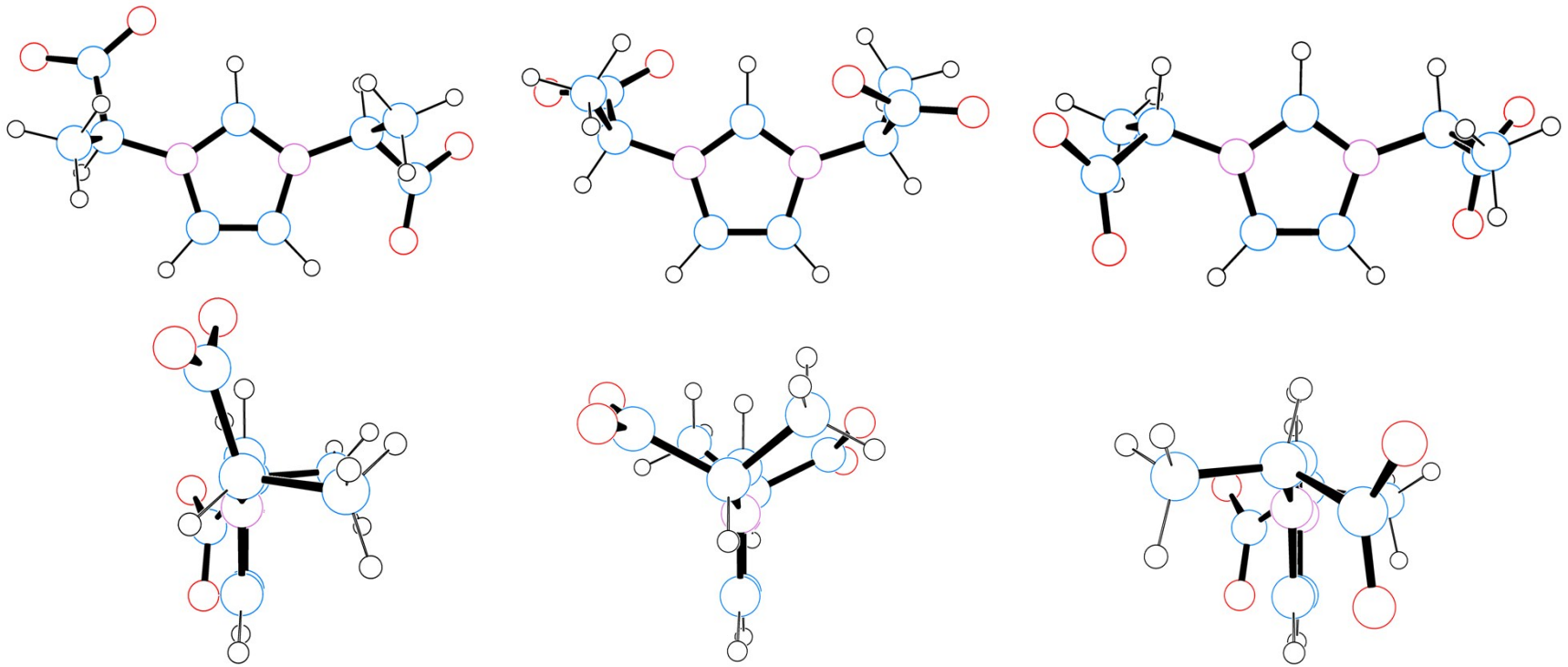


- **Table S3.** Comparison between selected experimental and theoretical structural parameters of compounds (*S*,*S*)-HL^{Me} and (*S*,*S*)-HL^{CH2Ph}.

Bond distances (Å) and angles (º)	**(*S*,*S*)-HL^{Me}**		**(*S*,*S*)-HL^{CH2Ph}**	
	Calculated	**X-ray LUYSAA**	**Calculated**	**X-ray LUYRON**
C-O (carboxylate)	1.232	1.207	1.231	1.205
	1.256	1.268	1.261	1.289
	1.202	1.221	1.200	1.214
	1.346	1.229	1.349	1.271
C=C (Im)	1.359	1.349(4)	1.360	1.361(7)
N-C (Im)	1.346	1.333(3)	1.348	1.330(8)
	1.330	1.329(3)	1.330	1.310(8)
	1.388	1.387(3)	1.388	1.340(10)
	1.384	1.370(3)	1.384	1.360(10)
O-C-O (carboxylate)	131.3	125.9	131.5	128.3
	124.3	125.9	123.9	128.4
N-C-N (Im)	108.6	108.6(2)	108.6	107.4(7)
C-N-C (Im)	108.6	108.1	108.6	109.4
	108.7	109.1	108.6	110.3
C-N-C_{chiral}	123.5	124.4(2)	122.6	123.8(6)
	126.2	125.8(2)	125.3	123.9(7)

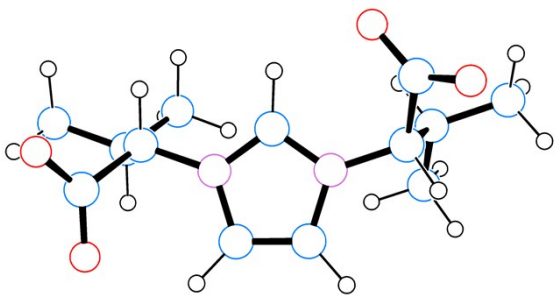
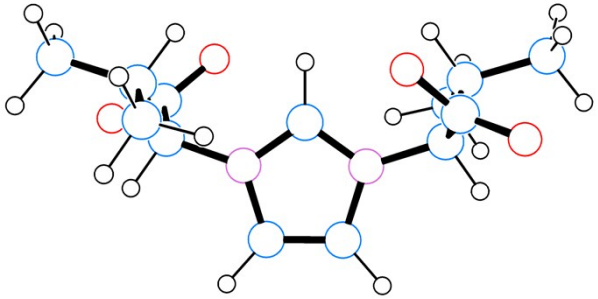
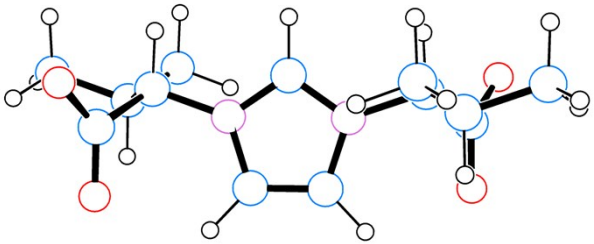
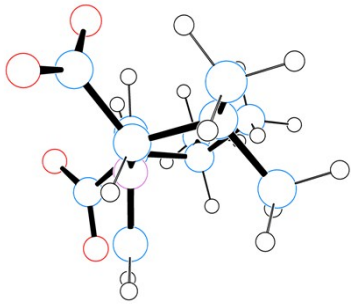
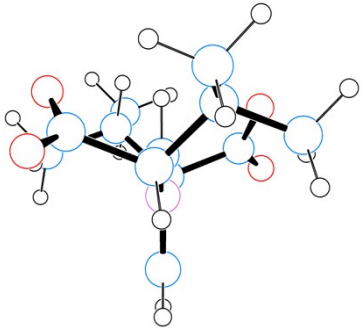
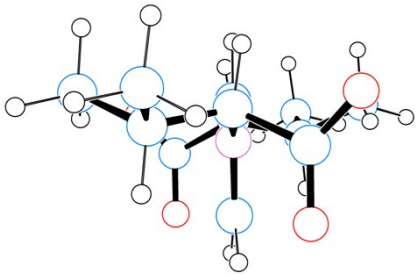
- Fig. S8. Optimised structures and energies (Hartree) of the three conformers of $[L^R]^-$ anions: frontal (up) and lateral views (bottom).

R = Me



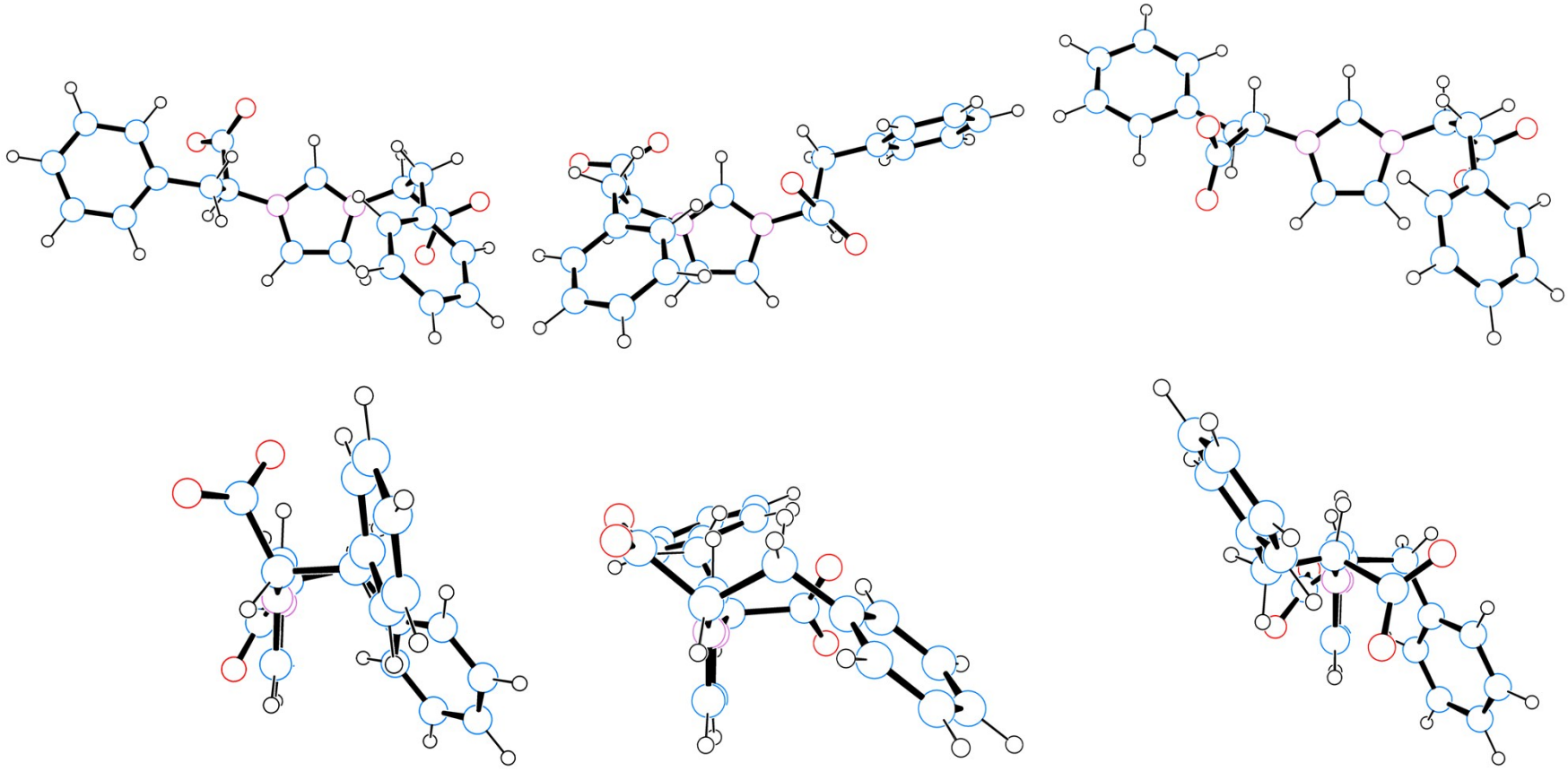
E	-760.29297465	-760.29070868	-760.29081021
Eo	-760.09403700	-760.09172500	-760.09186500
Et	-760.07938900	-760.07682300	-760.07706300
H	-760.07844500	-760.07587900	-760.07611900
G	-760.13832900	-760.13670600	-760.13725600

R = ^{i}Pr

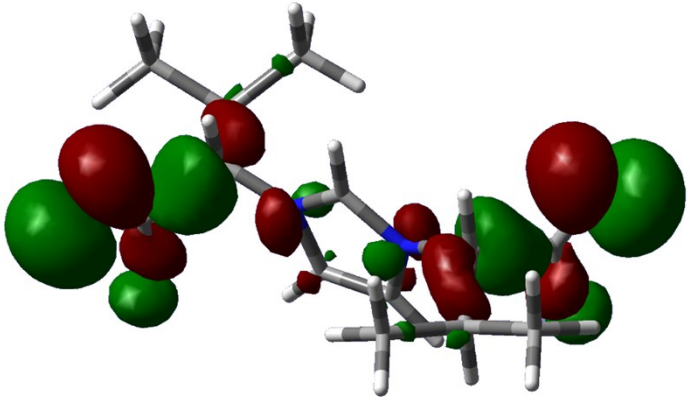
E	-917.587105947	-917.586526299	-917.587526567
Eo	-917.275621000	-917.275230000	-917.276280000
Et	-917.255576000	-917.254801000	-917.256016000
H	-917.254632000	-917.253857000	-917.255072000
G	-917.325688000	-917.327197000	-917.327330000

R = CH_2Ph

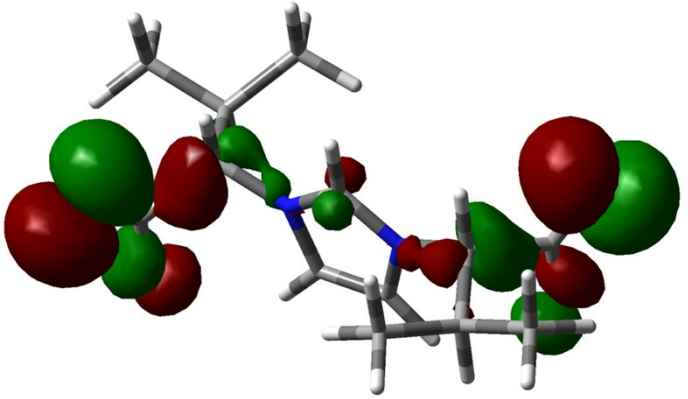


E	-1222.505047990	-1222.506069950	-1222.50357700
Eo	-1222.143510000	-1222.144399000	-1222.14203100
Et	-1222.120116000	-1222.120785000	-1222.11852000
H	-1222.119172000	-1222.119841000	-1222.11757600
G	-1222.201787000	-1222.202936000	-1222.20076800

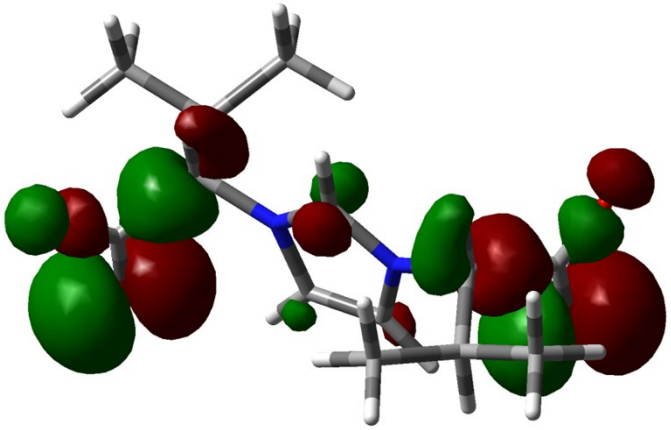
- Fig. S9. Computed HOMO to HOMO-3 of (*S*,*S*)-2,2'-(imidazolium-1,3-diyl)bis(3-methylbutanoate) anion, [(*S*,*S*)-L^{iPr}]$^-$, and their energies (eV).



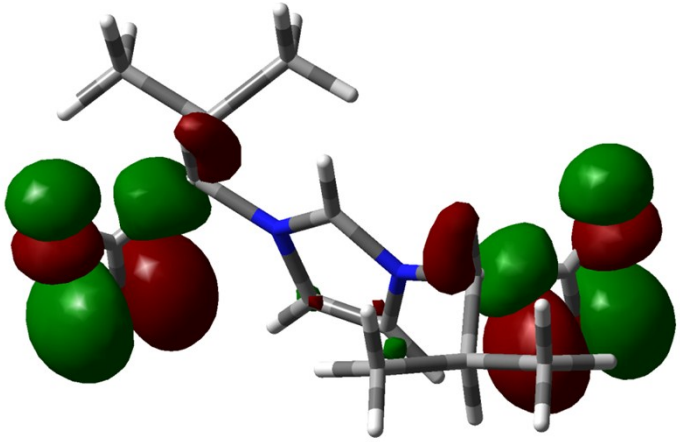
HOMO, -0.11097 eV



HOMO-1, -0.11475 eV



HOMO-2, -0.11719 eV



HOMO-3, -0.11824 eV

- Table S4. Coordinates of the optimised HL^R and $[L^R]^-$ compounds.

(*S*,*S*)-HL^{Me}

O	-3.22488400	0.14317800	-1.49512100
O	2.28626200	-1.88085900	0.43777000
O	4.24386600	-1.30209600	-0.55006100
N	-0.94060900	0.36093600	0.15775000
N	1.17845200	0.63304600	-0.24087100
C	0.28078400	-0.18815000	0.29752100
H	0.59049600	-1.14677000	0.70976000
C	0.51791300	1.74363400	-0.73701500
H	1.04167700	2.54344300	-1.23089900
C	-0.80890600	1.58000100	-0.49269000
H	-1.65438100	2.18806300	-0.75677500
C	-2.16833300	-0.26106000	0.66059800
H	-1.87716000	-1.23313900	1.05995200
C	-3.15966000	-0.49803500	-0.48114100
C	2.66164500	0.40740300	-0.30122500
H	2.95258100	0.71577300	-1.30615800
C	3.10215700	-1.11049300	-0.12727700
O	-3.99339500	-1.50661700	-0.16677100
H	-4.63473900	-1.60586600	-0.88801300
C	3.35569000	1.28293400	0.74395300
H	3.13334600	2.34692700	0.61152400
H	3.06067400	0.98628600	1.75403900
H	4.43119200	1.13572800	0.64406800
C	-2.82337600	0.57183400	1.77441400
H	-3.69908200	0.04830000	2.16010900
H	-2.11465100	0.71647800	2.59132100
H	-3.13714900	1.54964200	1.40355500

(*S*,*S*)-HL^{CH2Ph}

O	3.60366700	-1.91252100	1.53401400
O	-2.18239800	-2.25484000	-1.04689200
O	-3.45458600	-2.54285800	0.81297300
N	1.38831200	-0.86593400	0.16021700
N	-0.69789200	-0.49853500	0.65466100
C	0.11365200	-1.12151400	-0.19527900
H	-0.27532200	-1.74620000	-0.99317100
C	0.07278000	0.18264300	1.58021300
H	-0.37069600	0.74934600	2.38013300
C	1.37930300	-0.04246000	1.27783600
H	2.28117100	0.27442500	1.76598600
C	2.53497100	-1.37662300	-0.59394800
H	2.14674900	-2.18320200	-1.21985600
C	3.56343600	-2.01622500	0.33900100
C	-2.19122700	-0.52848500	0.60194000
H	-2.52613200	-0.39648000	1.63065900
C	-2.67018000	-1.94771700	0.07413300
O	4.44826800	-2.73295200	-0.38464300
C	-2.67326500	0.63226700	-0.29566000
H	-2.16571600	1.55569100	0.00700300
H	-2.36262300	0.40058100	-1.31875900
C	3.15937400	-0.32013600	-1.55378200
H	3.91257700	-0.84681800	-2.14396600
H	2.36646500	-0.01966300	-2.24303400
C	3.76487700	0.90165500	-0.89863500
C	5.07282300	0.87494800	-0.39888200
C	3.03305600	2.08956500	-0.79337100
C	5.62760300	2.00023900	0.20642800
H	5.66928100	-0.02617900	-0.49768000
C	3.58650100	3.21804100	-0.19128100
H	2.02561900	2.13628100	-1.19393800
C	4.88412500	3.17450000	0.31453300
H	6.64287000	1.96287800	0.58452900
H	3.00643900	4.13137300	-0.12378900
H	5.31727200	4.05228500	0.78006900
C	-4.16931200	0.85190600	-0.24228100
C	-5.04334000	0.02067400	-0.95224600

C	-4.70596700	1.89281800	0.52232100
C	-6.41908100	0.22795000	-0.89428500
H	-4.64369200	-0.79834500	-1.53971700
C	-6.08281600	2.10322000	0.58041900
H	-4.04024700	2.55081700	1.07358200
C	-6.94377500	1.26911600	-0.12940800
H	-7.08279400	-0.42947500	-1.44460800
H	-6.48041100	2.91710200	1.17694100
H	-8.01556300	1.42797200	-0.08629700
H	5.08096900	-3.13402700	0.23155500

[(*S*,*S*)-L^{Me}]$^{-}$ anion, conformer 1

O	-3.56916800	1.00224200	-0.80459500
O	2.52367600	-1.88128600	-0.09522400
O	4.39597900	-0.84156300	-0.84155600
N	-0.98079700	0.13805900	0.04973300
N	1.13827500	0.62066200	-0.13705000
C	0.26130900	-0.36456200	0.09056400
H	0.57394500	-1.38553200	0.24614100
C	0.42257200	1.79212600	-0.32228900
H	0.91386600	2.72458300	-0.53916700
C	-0.90125600	1.49485800	-0.20624000
H	-1.80921200	2.05928900	-0.33706500
C	-2.21056400	-0.66410200	0.31269900
H	-1.96433300	-1.67910100	0.00173100
C	-3.48861900	-0.21085300	-0.50919200
C	2.62812700	0.54131400	-0.15071800
H	2.94109400	1.17036600	-0.98534300
C	3.23462100	-0.89946400	-0.40545400
O	-4.28504000	-1.14679400	-0.69093400
C	3.18308200	1.10627300	1.16143600
H	2.84454400	2.13151600	1.34524800
H	2.87462200	0.48274800	2.00510700
H	4.27245200	1.09823600	1.10532700
C	-2.53047700	-0.63984100	1.81110600
H	-3.40032700	-1.27416000	1.98916600
H	-1.69278400	-1.01027100	2.41162000
H	-2.77256500	0.37599900	2.13546600

[(*S*,*S*)-L^{Me}]$^{-}$ anion, conformer 2

O	-2.27424500	-1.43071300	-1.00879400
O	2.27358600	1.43760800	-0.99910800
O	4.31168700	0.59247200	-0.44714900
N	-1.03526700	0.33793400	0.70013800
N	1.03542500	-0.34328000	0.69774400
C	0.00018200	0.00038000	-0.07629900
H	0.00046900	0.00479800	-1.14705300
C	0.64747900	-0.21708900	2.01729100
H	1.32351900	-0.42602600	2.82742500
C	-0.64771500	0.20129300	2.01874300
H	-1.32401100	0.40391000	2.83026600
C	-2.40475200	0.63155100	0.23209100
H	-2.98089200	0.84379600	1.13350300
C	-3.06792800	-0.62441100	-0.48659000
C	2.40502400	-0.63302900	0.22759900
H	2.98128100	-0.85133500	1.12748500
C	3.06763700	0.62823000	-0.48222500
O	-4.31196900	-0.58808900	-0.45160000
C	2.42403900	-1.84510700	-0.70560200
H	2.00870200	-2.73619100	-0.22480200
H	1.85317300	-1.64978000	-1.61663600
H	3.45912400	-2.03930200	-0.99034100
C	-2.42334400	1.85017600	-0.69257600
H	-3.45848700	2.04733400	-0.97503700
H	-2.00667400	2.73744200	-0.20591500
H	-1.85352300	1.66058700	-1.60545200

[(*S*,*S*)-L^{Me}]$^{-}$ anion, conformer 3

O	3.42014900	-0.68320100	1.27034400
O	-3.42221700	0.66752000	1.27714600
O	-4.41731500	0.88576400	-0.75430900
N	1.07925600	0.17373400	-0.11173400
N	-1.07945100	-0.17290900	-0.11348400
C	-0.00004900	0.00395600	-0.88419000
H	0.00004100	0.00881100	-1.96007400
C	-0.67453500	-0.11241500	1.20639200
H	-1.40315600	-0.17269900	1.99459400
C	0.67414100	0.10114000	1.20746900
H	1.40257200	0.15406900	1.99635700
C	2.44855700	0.43062800	-0.62467200
H	2.40939500	0.19377300	-1.68854100
C	3.54629400	-0.50211300	0.04154400
C	-2.44878700	-0.42506200	-0.62895900
H	-2.40947400	-0.17836500	-1.69058400
C	-3.54607700	0.50185200	0.04589100
O	4.42013600	-0.87409100	-0.76146000
C	-2.81895700	-1.89831800	-0.44230400
H	-2.09623100	-2.56492900	-0.92497700
H	-2.87192200	-2.14669200	0.62006100
H	-3.80405300	-2.06888000	-0.88149400
C	2.81881000	1.90212900	-0.42446300
H	3.80379600	2.07658100	-0.86230400
H	2.09594800	2.57321600	-0.90068200
H	2.87204600	2.14062600	0.64015500

[(*S*,*S*)-L^{iPr}]$^{-}$ anion, conformer 1

O	3.56926500	-0.96759700	1.53123400
O	-2.28250900	-1.15410600	-1.90013700
O	-3.85865900	-2.13663200	-0.59368100
N	1.04405600	-0.26068600	0.29945100
N	-1.11632300	-0.33650500	0.59780900
C	-0.14298400	-0.29919500	-0.32208800
H	-0.34048500	-0.35148400	-1.38031800
C	-0.52173700	-0.32652500	1.84711300
H	-1.10673000	-0.37194600	2.74859000
C	0.82756800	-0.27881500	1.66550500
H	1.67191000	-0.31609600	2.33378400
C	2.36246700	-0.17849100	-0.38329200
H	2.18601600	-0.52307500	-1.40368900
C	3.42203500	-1.14441900	0.29862700
C	2.88128300	1.27925100	-0.39175500
H	3.03931900	1.55559800	0.65708000
C	1.88952300	2.26775200	-1.02185800
H	2.30028100	3.28233300	-1.00211700
H	0.93284500	2.29291600	-0.49369800
H	1.68881700	2.01340000	-2.06885800
C	4.23739400	1.35077700	-1.10903300
H	4.14148700	1.05036800	-2.15792500
H	4.97199100	0.69241700	-0.64416400
H	4.62179300	2.37563700	-1.08524800
C	-2.57890600	-0.35264200	0.33450000
H	-3.03368500	-0.73193200	1.25167200
C	-2.93908300	-1.34303500	-0.84954300
C	-3.09969100	1.07364800	0.03315600
H	-2.59586300	1.39535800	-0.88575300
C	-2.78013600	2.07844400	1.14999900
H	-3.15262400	3.07306900	0.88464000
H	-1.70734800	2.16815700	1.33731400
H	-3.26344600	1.78672200	2.09004800
C	-4.60995700	1.04194900	-0.24172100
H	-4.85320100	0.37614800	-1.07010400
H	-4.96871600	2.04777300	-0.48298300
H	-5.16014200	0.68825500	0.63688400
O	4.00277700	-1.90860000	-0.48787200

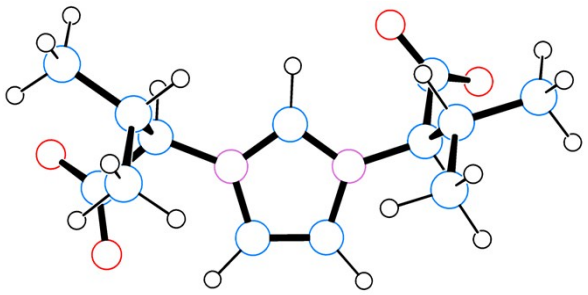
[(*S*,*S*)-L^{iPr}]$^{-}$ anion, conformer 2

O	-1.86380100	-1.92581700	-0.98420500
O	1.86395300	1.92585300	-0.98430800
O	3.82869000	2.01134700	0.15586700
N	-1.08877900	0.04992700	0.82824800
N	1.08877800	-0.04998500	0.82822200
C	-0.00000600	0.00007200	0.05129400
H	0.00000600	0.00027200	-1.01945300
C	0.68004900	-0.02877900	2.14733000
H	1.38762800	-0.04366300	2.95716200
C	-0.68004200	0.02826500	2.14734700
H	-1.38761500	0.04287700	2.95718900
C	-2.48743900	-0.04707600	0.36279700
H	-3.10372000	0.09115600	1.25364500
C	-2.75352200	-1.50612200	-0.21629700
C	2.48743700	0.04709800	0.36277100
H	3.10369800	-0.09119500	1.25362200
C	2.75352400	1.50619500	-0.21620000
O	-3.82880600	-2.01120400	0.15553200
C	2.81488700	-1.05393700	-0.66939900
H	2.18570400	-0.86951700	-1.54764900
C	-2.81486500	1.05402600	-0.66930000
H	-2.18563600	0.86969000	-1.54753500
C	-4.28002100	0.94589000	-1.11501800
H	-4.49298600	1.69675200	-1.88248300
H	-4.50889700	-0.04223900	-1.51505000
H	-4.95723500	1.12277200	-0.27215800
C	-2.51025200	2.46329100	-0.13902900
H	-3.10952000	2.68187700	0.75309900
H	-1.45564000	2.59284600	0.11359900
H	-2.75746600	3.21465700	-0.89534300
C	4.28006900	-0.94585900	-1.11504200
H	4.49304300	-1.69671900	-1.88250600
H	4.50900900	0.04226500	-1.51504900
H	4.95723500	-1.12277800	-0.27215100
C	2.51015800	-2.46321800	-0.13924500
H	3.10935500	-2.68189900	0.75290900
H	1.45551900	-2.59271500	0.11330300
H	2.75737400	-3.21455100	-0.89559000

[(*S*,*S*)-L^{iPr}]$^{-}$ anion, conformer 3

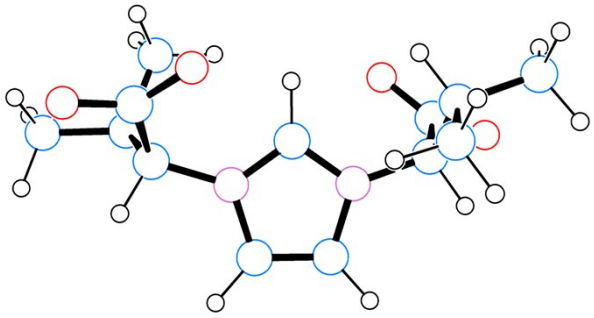
O	-3.26080000	1.37940000	1.47570000
O	3.26080000	-1.37940000	1.47570000
O	3.69690000	-2.17980000	-0.60590000
N	-1.09100000	0.06040000	0.08570000
N	1.09100000	-0.06040000	0.08570000
C	0.00000000	0.00000000	-0.68670000
H	0.00000000	0.00000000	-1.76210000
C	0.68130000	-0.04070000	1.40580000
H	1.40600000	-0.14180000	2.19410000
C	-0.68130000	0.04060000	1.40580000
H	-1.40600000	0.14160000	2.19410000
C	-2.48630000	0.13020000	-0.40950000
H	-2.40880000	0.28540000	-1.48810000
C	-3.22690000	1.38430000	0.22580000
C	2.48630000	-0.13020000	-0.40960000
H	2.40880000	-0.28530000	-1.48810000
C	3.22690000	-1.38420000	0.22570000
O	-3.69680000	2.17990000	-0.60580000
C	3.23810000	1.18620000	-0.11730000
H	3.27840000	1.28570000	0.97310000
C	-3.23820000	-1.18620000	-0.11730000
H	-3.27860000	-1.28560000	0.97300000
C	-4.68020000	-1.08970000	-0.63480000
H	-5.22540000	-2.01110000	-0.40740000
H	-5.21160000	-0.25180000	-0.18140000
H	-4.69840000	-0.94680000	-1.72090000
C	-2.53030000	-2.41530000	-0.70480000
H	-2.47330000	-2.35110000	-1.79800000
H	-1.51430000	-2.53540000	-0.32030000
H	-3.08240000	-3.32780000	-0.45900000

C	2.53030000	2.41530000	-0.70490000
H	2.47340000	2.35110000	-1.79810000
H	1.51430000	2.53540000	-0.32050000
H	3.08230000	3.32780000	-0.45910000
C	4.68020000	1.08970000	-0.63470000
H	5.21150000	0.25190000	-0.18110000
H	4.69850000	0.94670000	-1.72070000
H	5.22530000	2.01120000	-0.40720000



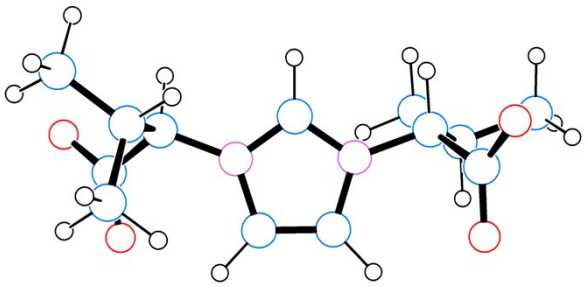
[(*R*,*R*)-L^{iPr}]$^{-}$ anion, conformer 1

O	-3.99969000	-2.11904000	0.09266300
O	3.51196000	-0.35983200	-1.75429700
O	4.34709600	-1.55248800	-0.01926500
N	-1.17750400	-0.20708600	-0.65647300
N	0.98633800	-0.29804000	-0.37654700
C	-0.20187900	-0.41175300	0.23629100
H	-0.39920300	-0.68976400	1.25868800
C	0.76493100	-0.01328200	-1.71208400
H	1.61200200	0.08662600	-2.37117600
C	-0.58600700	0.04202900	-1.88225500
H	-1.17469400	0.22647700	-2.76338600
C	-2.63727800	-0.22071900	-0.38392800
C	-3.03947800	-1.45900700	0.52118300
C	2.29228100	-0.44727000	0.33897500
C	3.50794400	-0.84237900	-0.59856000
O	-2.36523800	-1.57298100	1.57134300
C	-3.08721400	1.10727500	0.27104400
H	-2.58335600	1.15513600	1.24350300
C	-4.60183500	1.08988900	0.52185600
H	-4.91095300	2.01548500	1.01805800
H	-5.15256200	1.01266000	-0.42193400
H	-4.89760400	0.24458600	1.14385300
C	-2.69434600	2.34433300	-0.55009200
H	-3.17806100	2.33185400	-1.53396000
H	-3.01463900	3.25756600	-0.03852700
H	-1.61531800	2.41567000	-0.70662900
H	-3.11264500	-0.33669700	-1.35985900
C	2.57774000	0.83815500	1.16394300
H	1.66120300	1.04574300	1.73518100
C	3.70480900	0.59696300	2.17751800
H	3.85360300	1.49242200	2.79016800
H	3.46678300	-0.23713100	2.84363500
H	4.64038600	0.35013600	1.67284500
C	2.86970600	2.06525200	0.28899800
H	2.05483800	2.26909000	-0.41089100
H	2.99883300	2.95140600	0.91929200
H	3.77755300	1.91863700	-0.30004600
H	2.14272900	-1.27620900	1.03143900



[(*R*,*R*)-L^{iPr}]$^{-}$ anion, conformer 2

O	3.74090000	-2.13983100	-0.02907200
O	-1.71667400	1.84896100	-1.08055700
O	-3.90253600	1.78480800	-0.47828500
N	1.12665300	-0.00562600	0.88600600
N	-1.05255200	0.05037300	0.91710100
C	0.02910100	0.11255400	0.12868500
H	0.00455200	0.26652500	-0.93030300
C	-0.62634700	-0.12902100	2.21995200
H	-1.32210800	-0.20560200	3.03680600
C	0.73379100	-0.16400000	2.20048200
H	1.45034700	-0.29205500	2.99241100
C	2.51150500	-0.13777000	0.38799300
C	2.68451700	-1.55079700	-0.32539500
C	-2.47040300	0.18077500	0.50267500
C	-2.71162900	1.42090900	-0.46259200
O	1.75545400	-1.85480000	-1.09961500
C	2.88795800	1.03666800	-0.54048800
H	2.21998500	0.99128700	-1.40810900
C	4.32642600	0.87621500	-1.05231900
H	4.57029500	1.69259400	-1.73963200
H	5.04183600	0.90612200	-0.22328400
H	4.46727900	-0.07322500	-1.56938700
C	2.70616000	2.39980900	0.14486900
H	3.35765600	2.48218300	1.02319200
H	2.97072700	3.20976900	-0.54176400
H	1.67546200	2.56866100	0.46483600
H	3.14605600	-0.11885500	1.27677200
C	-3.00011900	-1.16754500	-0.06186300
H	-2.62558700	-1.94883300	0.61501900
C	-4.53465300	-1.21066300	-0.01399500
H	-4.89193800	-2.18638500	-0.35990700
H	-4.90417200	-1.05648700	1.00536100
H	-4.96323300	-0.42502700	-0.63773200
C	-2.47977500	-1.48466900	-1.47113200
H	-1.39129500	-1.57373900	-1.50303400
H	-2.88993300	-2.44104900	-1.81096900
H	-2.78290900	-0.71107100	-2.18159300
H	-3.00807200	0.39407900	1.42857000



[(*R*,*R*)-L^{iPr}]$^{-}$ anion, conformer 3

O	-3.70140200	-2.19461300	-0.74804300
O	3.16617400	1.18608700	1.62635800
O	4.20746200	1.79130600	-0.29528800
N	-1.14924000	-0.05390100	0.06120200
N	1.02915000	0.14837800	0.06615500
C	-0.06410600	0.08974600	-0.70603600
H	-0.07010600	0.15201200	-1.77992800
C	0.62342300	0.03412900	1.38381400
H	1.35211400	0.11288600	2.17075800
C	-0.73580000	-0.09548400	1.37966100
H	-1.45375100	-0.26731700	2.16200600
C	-2.54295700	-0.12908800	-0.43688300
C	-3.25526900	-1.43287700	0.12724500
C	2.41071100	0.26871200	-0.47853700
C	3.35525200	1.19975300	0.39214200
O	-3.29582000	-1.49369200	1.37528600
C	-3.32616600	1.15023500	-0.07105000
H	-3.37804600	1.17998700	1.02280400
C	-4.76091200	1.05450100	-0.60865800
H	-5.33062100	1.94530700	-0.32578100
H	-4.76622700	0.98420400	-1.70200200
H	-5.27533900	0.17574000	-0.21745700
C	-2.64154900	2.42959300	-0.57272700
H	-2.56309800	2.43139300	-1.66654300
H	-3.22231300	3.31154300	-0.28487000
H	-1.63642000	2.55237000	-0.16116400
H	-2.46320600	-0.22204500	-1.52246200
C	3.01576400	-1.14180400	-0.72398500
H	2.23557800	-1.72627700	-1.23338500
C	4.22090700	-1.05083500	-1.67153200
H	4.61615800	-2.05224500	-1.87137500
H	3.94238300	-0.59824700	-2.62830000
H	5.01031700	-0.43359400	-1.23941800
C	3.38484800	-1.88396600	0.56773900
H	2.52309500	-2.00555800	1.22806200
H	3.76179100	-2.88326700	0.32710200
H	4.15530100	-1.34440800	1.12309200
H	2.28684900	0.75779600	-1.44629500

[(*S*,*S*)-L^{CH2Ph}]$^{-}$ anion, conformer 1

O	3.93385600	-1.85907900	1.57980200
O	-2.11215900	-2.05736200	-1.48778100
O	-3.34517400	-2.81903100	0.26057400
N	1.55451200	-1.15754100	0.25715600
N	-0.56399000	-0.89008300	0.70267000
C	0.30930200	-1.32480300	-0.21195900
H	0.00035900	-1.74294900	-1.15766400
C	0.15349900	-0.42207100	1.78994300
H	-0.33780800	-0.03589700	2.66561700
C	1.47692700	-0.58948200	1.51481300
H	2.36880200	-0.43420000	2.09363500
C	2.78004400	-1.47022700	-0.52699500
H	2.53307500	-2.36525100	-1.10178800
C	4.05738200	-1.85484500	0.34100700
C	-2.04289000	-0.83782200	0.56085900
H	-2.44396600	-0.93639700	1.56990100
C	-2.55975800	-2.05311100	-0.31287100

O	5.03872600	-2.10527000	-0.38321300
C	-2.42546600	0.52642400	-0.05596100
H	-1.90596000	1.32415500	0.48633800
H	-2.05354600	0.52300400	-1.08443500
C	3.08208800	-0.33563600	-1.53503000
H	3.94166200	-0.69061200	-2.10640400
H	2.23827200	-0.23313400	-2.22619500
C	3.39009600	1.01476500	-0.92462900
C	4.62136000	1.25572200	-0.29781500
C	2.45659400	2.05580700	-0.97883300
C	4.90117700	2.50115800	0.25951800
H	5.34986400	0.45410100	-0.24498100
C	2.73559000	3.30432900	-0.42248100
H	1.50120400	1.88902000	-1.46738300
C	3.96105700	3.53070400	0.20029300
H	5.85812800	2.66733100	0.74312600
H	1.99647100	4.09693100	-0.47731200
H	4.18286900	4.50009300	0.63434000
C	-3.91212500	0.80481400	-0.04454600
C	-4.76463300	0.19683400	-0.97510300
C	-4.46778000	1.67659600	0.89811500
C	-6.13246100	0.45816700	-0.95945200
H	-4.34898800	-0.49527600	-1.69916400
C	-5.83707400	1.94047500	0.91559100
H	-3.81975400	2.15897500	1.62424900
C	-6.67476000	1.33121400	-0.01627200
H	-6.77773200	-0.02796100	-1.68332000
H	-6.24674100	2.62124200	1.65471100
H	-7.74087600	1.53206300	-0.00625000

[(*S*,*S*)-L^{CH2Ph}]$^{-}$ anion, conformer 2

O	-0.89121700	-1.57164100	-0.94529300
O	1.33395800	3.44463700	-0.68911800
O	3.57549000	3.80880400	-0.57378600
N	-0.42556800	0.38909000	1.08156000
N	1.60800600	1.09276900	0.74068500
C	0.39592900	0.95965600	0.19248700
H	0.13689300	1.28188700	-0.79586800
C	1.55949500	0.59098800	2.02583800
H	2.42516500	0.58766800	2.66394500
C	0.29068700	0.14800800	2.24001000
H	-0.15777200	-0.33872500	3.08783800
C	-1.75796400	-0.17343000	0.78620500
H	-2.25864500	-0.29487100	1.74714300
C	-1.53460400	-1.61087900	0.12651100
C	2.78522000	1.67720800	0.07116000
H	3.57016600	1.71080600	0.82688600
C	2.52330200	3.15866200	-0.44557000
O	-2.02224500	-2.55874900	0.76207100
C	3.23867700	0.78545000	-1.10787700
H	2.44444600	0.77069200	-1.85975000
H	4.09294000	1.29860200	-1.55478100
C	-2.55332200	0.77720400	-0.12498000
H	-2.47830400	1.79916000	0.26075500
H	-2.09058500	0.75902100	-1.11521700
C	3.61080100	-0.62789700	-0.71686700
C	2.66605100	-1.66301200	-0.74620200
C	4.91063700	-0.92232600	-0.28352700
C	3.01393000	-2.95285500	-0.34414200
H	1.64645900	-1.47597600	-1.07248900
C	5.26075000	-2.21171400	0.11282600
H	5.65512000	-0.13154100	-0.26322000
C	4.31016600	-3.23273600	0.08538100
H	2.26079100	-3.73265700	-0.36716200
H	6.27491100	-2.41962700	0.43913300
H	4.57884400	-4.23748100	0.39472300
C	-4.01157500	0.39167700	-0.24662500
C	-4.99484600	1.08736100	0.46483900
C	-4.40913100	-0.66760400	-1.07185200
C	-6.34123800	0.73984100	0.35841800
H	-4.70298400	1.91545400	1.10393500
C	-5.75275100	-1.01813600	-1.17864000

H	-3.65660100	-1.22397300	-1.61944900
C	-6.72469700	-0.31621100	-0.46573700
H	-7.08793000	1.29544200	0.91640400
H	-6.04017400	-1.84605100	-1.81794800
H	-7.77081800	-0.59078100	-0.55151700

[(*S*,*S*)-L^{CH2Ph}]$^{-}$ anion, conformer 3

O	2.30701100	2.32922700	-0.85450300
O	-2.93756100	-2.43123500	-1.50629300
O	-4.22616800	-3.13487200	0.22513800
N	0.68533500	-0.09193700	-0.03387500
N	-1.32708300	-0.91886300	0.15851700
C	-0.11353300	-0.84980500	0.72146800
H	0.17341500	-1.32259200	1.64417700
C	-1.29943000	-0.17643400	-1.00515700
H	-2.15615400	-0.12725900	-1.64972900
C	-0.04563100	0.34806400	-1.12255700
H	0.39653900	1.01743100	-1.83964700
C	2.10189100	0.22329500	0.25848100
H	2.29318700	-0.15919200	1.26180700
C	2.25400600	1.80967400	0.28276200
C	-2.47938100	-1.64399900	0.74021200
H	-2.04315700	-2.36869200	1.43211800
C	-3.30273900	-2.50055400	-0.32077300
O	2.27588600	2.30758400	1.41877100
C	-3.38164500	-0.69860300	1.56796700
H	-2.79063900	-0.25244700	2.37573900
H	-4.12731400	-1.35493800	2.02098700
C	3.00569900	-0.46925900	-0.77827300
H	2.69154400	-1.51261200	-0.89332100
H	2.85168600	0.03986900	-1.73283600
C	-4.07092300	0.40340200	0.79174100
C	-5.16642200	0.12014600	-0.03649900
C	-3.63088100	1.72820700	0.88706200
C	-5.79706600	1.13805700	-0.74807100
H	-5.50710800	-0.90555200	-0.12671400
C	-4.26187700	2.74855400	0.17545400
H	-2.78216800	1.96559000	1.52114400
C	-5.34899900	2.45562900	-0.64501500
H	-6.63985900	0.89970200	-1.38847600
H	-3.89885100	3.76725200	0.25980100
H	-5.84125500	3.24586300	-1.20216200
C	4.47196600	-0.42855800	-0.40470200
C	5.22396200	0.74368800	-0.56025000
C	5.10697000	-1.56461700	0.10974700
C	6.57187800	0.77150600	-0.20942100
H	4.73502400	1.63258600	-0.94354800
C	6.45658500	-1.53870400	0.46059200
H	4.53917000	-2.48268300	0.23064700
C	7.19461000	-0.36765900	0.30111600
H	7.13685000	1.68956800	-0.33192000
H	6.92923900	-2.43207400	0.85571500
H	8.24452500	-0.34203900	0.57351600